Fundamental Properties of Polymer Nanocomposites from Molecular Simulation

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The emerging field of nanotechnology requires quantification of material properties at length scales that are difficult to probe experimentally, but ideally suited to molecular simulation methods. We present results of simulations focused on fundamental properties of polymer nanocomposites that are also industrially relevant. Controlling nanoparticle dispersion in composite materials is critical to obtain improvements in bulk properties. We characterize the factors controlling dispersion in a model nanoparticle composite and show that dispersion can occur via a variety of mechanisms, with a focus on thermo-reversible gelation. We subsequently show how the state of dispersion affects rheological properties, important to material processing. Additionally, we consider the role of nanoparticle geometry on bulk properties, emphasizing the importance of the surface-to-volume ratio of nanoparticles. We link these simulations to ongoing experiments to help show how molecular simulation can aid the study of real systems.